Abstract Submitted
for the MAS20 Meeting of
The American Physical Society

Tuning Polarization and Electronic Structure via Chemical Substitution in Two Dimensional Ferroelectrics JOSHUA YOUNG, MO LI, OLAMIDE OMISAKIN, New Jersey Institute of Technology — Two dimensional materials with switchable spontaneous electric polarizations ("2D ferroelectrics") have recently been garnering attention as components for ultrathin electronic devices. However, 2D ferroelectrics with out-of-plane polarizations are challenging to find. Recently, Chandrasekaran et al. proposed that the functionalized MXene Sc_2CO_2 has a metastable state with a large out-of-plane polarization. [1] In this work, we used density functional theory (DFT) calculations to investigate additional M_2CX_2 materials (M = Sc, Y, La; X = O, F). We found that (1) substitution of Sc with Y and/or O with F can stabilize the ferroelectric phase as the ground state (the dynamic stability was verified with phonon calculations); (2) substitution can also be used to tune the polarization and band gap; and (3) these monolayers display large piezoelectric coefficients. We also show that these properties can be continuously tuned by the application of external strain or by alloying to create $Sc_{2x}Y_{2(1-x)}CO_2$ monolayers. These findings demonstrate that chemical substitution and external stimuli are powerful ways to stabilize and control the properties of low dimensional ferroelectric materials. [1] A. Chandrasekaran, A. Mishra, A. K. Singh, Nano Letters 17 3290 (2017)

Joshua Young
New Jersey Institute of Technology

Date submitted: 02 Nov 2020 Electronic form version 1.4